

Self-similar solutions and collective coordinate methods for Nonlinear Schrödinger Equations

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Abstract

In this paper we study the phase of self-similar solutions to general Nonlinear Schrödinger equations. From this analysis we gain insight on the dynamics of non-trivial solutions and a deeper understanding of the way collective coordinate methods work. We also find general evolution equations for the most relevant dynamical parameter $w(t)$ corresponding to the width of the solution. These equations are exact for self-similar solutions and provide a shortcut to find approximate evolution equations for the width of non-self-similar solutions similar to those of collective coordinate methods.

Key words: Nonlinear Schrödinger equations, collective coordinate methods, self-similar solutions, time-dependent variational method, Nonlinear Optics, Nonlinear matter waves, solitary waves

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1 Introduction

The nonlinear Schrödinger equation (NLSE) in its many versions is one of the most important models of mathematical physics, with applications to different fields such as plasma physics, nonlinear optics, water waves and biomolecular dynamics, to cite only a few cases. In many of those examples the equation appears as an asymptotic limit for the slowly varying envelope of a dispersive wave propagating in a nonlinear medium [1,2]. A new burst of interest on nonlinear Schrödinger equations has been triggered by the experimental achievement of Bose-Einstein condensation (BEC) using ultracold neutral bosonic gases [3,4].

Many different forms of the Nonlinear Schrödinger equation appear in practical applications but many of them are included in the following family of equations

$$i\frac{\partial u}{\partial t} = -\frac{1}{2}\Delta u + V(x, t)u + g(|u|^2; t)u, \quad (1)$$

where $u(x, t)$ is a complex function to be determined, $x \in \Omega \subset \mathbb{R}^n$, $V(x, t)$ is a real function called the *potential* and g is a real function satisfying $g(y; t) \rightarrow 0, y \rightarrow 0$ accounting for the nonlinearities. In many physical applications $\Omega \equiv \mathbb{R}^n$ and u has at least finite L^2 and H^1 norms in the spatial variables because of its physical meaning of *mass* and *energy* of the solutions. Most of the results to be presented in this paper can be extended without problems to the so-called vector case, when $u = (u_1, \dots, u_M)$, however, to keep the formalism as simple as possible we concentrate here on the scalar case.

Many questions may be posed from the mathematical point of view on the properties of solutions of Eqs. (1). Results are available for local and global existence, asymptotic behavior, etc ... [2,5,6]. In some very restricted one dimensional situations it is even possible to find the analytical expression of the solutions by the use of the so-called inverse scattering transform or equivalent methods [7]. Finally, the so-called moment method allows in some specific cases to obtain rigorous results for the evolution of integral quantities related to the solution of Eq. (1) [8,9,10].

However, very little is known (rigorously) on the dynamics of solutions which are asymptotically non-stationary (e.g. when either the conditions discussed in Refs. [5,6] do not hold or there are more complex non-autonomous situations, etc).

For those situations it is customary in the applied sciences to use the so called time-dependent variational method, collective coordinates method or averaged-Lagrangian method [11,12] to obtain some insight on the behavior of the solutions. All of the names refer to the same idea, which consists on rewriting Eq. (1) as a variational problem on the basis of the Lagrangian density so that the problem of solving Eq. (1) is transformed into the one of finding $u(x, t)$ such that the action

$$S = \int \mathcal{L}(u, u^*, \nabla u, \nabla u^*, x, t) d^n x dt \quad (2)$$

be one extremum. Of course, this problem is in principle as complicated as that of solving the original nonlinear Schrödinger equation (1). The idea of the method of collective coordinates is to restrict the analysis to a specific family of functions, that is to find the extremum of (2) over a specific family of functions $u(x, t) = \varphi(x, q_1(t), \dots, q_K(t); t)$ with fixed φ and letting $q_1(t), \dots, q_K(t)$ be unknown functions containing the dynamics of φ . Once the test function is chosen one may explicitly compute an averaged Lagrangian

$$L(t) = \int \mathcal{L}(\phi, \phi^*, \nabla \phi, \nabla \phi^*, x, t) d^n x, \quad (3)$$

and the problem becomes a finite-dimensional one for the unknowns q_1, \dots, q_K . Thus, the evolution equations for the parameters are obtained by solving the Euler-Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0, j = 1, \dots, K. \quad (4)$$

The accuracy of the results depends crucially on the proper choice of the family of test functions φ . In practice, this choice requires some knowledge of the solution obtained either from numerical simulations, asymptotic behaviors, or on the basis of more or less heuristic reasoning. Also the type of solutions studied usually have a simple form to keep the complexity of the calculations under control.

There is an immense body of references on the application of the collective coordinate method to many specific applications, normally from a heuristic perspective. Two panoramas for its application in different fields can be seen in [11] and [12].

One drawback of the method is that in the framework of Nonlinear Schrödinger systems it is usually possible to guess an approximate form for the amplitude of the solution, but the choice of the phase is more difficult to justify. Usually a simple form is chosen based on the experience of the linear Schrödinger equations as will be discussed later.

In this paper we propose a way to choose the phase systematically by solving exactly the phase equation corresponding to self-similar solutions. We also discuss how to use this phase to construct simple evolution equations for the parameters which improve the variational equations. In this analysis it will be also clear why the usual form of the method of collective coordinates is able to provide reasonable results for the dynamics.

2 Formulation of the problem

We start our analysis from Eq. (1) and split u into amplitude and phase by writing $u(x, t) = a(x, t)e^{i\phi(x, t)}$. After substitution in Eq. (1) we obtain the following coupled system of equations

$$\frac{\partial a}{\partial t} = -(\nabla a)(\nabla \phi) - \frac{1}{2}a\Delta \phi, \quad (5a)$$

$$\rho \frac{\partial \phi}{\partial t} = \frac{1}{2}\Delta a - \frac{1}{2}(\nabla \phi)^2 a - V(x, t)a - g(a, t)\rho. \quad (5b)$$

From now on we concentrate on non-propagating solutions of Eq. (1), i.e., those for which the “centrum” of the wavepacket defined as $X_j(t) = \int x_j(a(x,t))^2 d^n x$ satisfies $X_j(t) = 0$. Because of the Ehrenfest theorem [13,14], for any type of nonlinear term g and for quadratic polynomial potentials, the evolution of this quantity can be decoupled exactly from the “internal” dynamics of the solution so that starting from solutions $u(x,t)$ with $X_j(t) \neq 0$ we may construct new solutions $u(x - X_j(t), t)$ satisfying $X_j(t) = 0$ as discussed in [14]. Thus for the above mentioned type of problems (which include many problems of practical interest) we may concentrate on the analysis of this type of solutions without loss of generality. For nonlinear Schrödinger equations with algebraic potentials or polynomial potentials of degree higher than two our analysis will be applicable to non-propagating solutions.

2.1 The phase of self-similar radially symmetric solutions

As discussed above, the key idea of the method of collective coordinates is to restrict the analysis to a particular set of functions $\varphi(x, q_1(t), \dots, q_M(t); t)$. In this paper we will call quasi-solutions to these functions which are not true solutions of the original equations (1) but in some sense provide some estimates for the dynamics provided the parameters $q_j(t)$ are chosen optimally and the choice of the set of trial functions is appropriate. In the case of Schrödinger equations, the time-dependent variational method proceeds usually by choosing quasi-solutions of the form

$$\varphi = A(t)\rho(r/w(t))e^{i\beta(t)r^2}. \quad (6)$$

Thus, when non-propagating symmetric systems are considered there appear usually three free parameters $A(t), w(t), \beta(t)$ to be determined (they have the physical meaning of amplitude, width and chirp of the solution) once the motion of the center has been decoupled. The consideration of non-symmetric systems over n spatial dimensions leads to $2n + 1$ independent parameters and can be handled in a similar way. The specific choice for the phase $\beta(t)r^2$ is believed to be a good one on the basis of what it happens in linear systems and previous experience with the equation. In fact, this term is chosen to be quadratic by analogy with the Optics of gaussian beams, ruled by linear Schrödinger equations. In that field it is well known that gaussian beams must include a quadratic phase term to be exact solutions of the linear propagation equations. One of the results of this paper will be to provide an understanding of why this approximation works so well for the nonlinear case.

The main point of our analysis is to study self-similar solutions of the form

$$u(x, t) = A(t)\rho(r/w(t))e^{i\phi(r,t)}. \quad (7)$$

being $A(t)$, $w(t)$, ρ and $\phi(r, t)$ real functions.

When self-similar solutions to Eq. (1) exist our Eq. (7) will provide exact solutions. When self-similar solutions do not exist we will understand Eq. (7) as an ansatz approximating the true solutions in a sense similar to that of the quasi-solutions of the method of collective coordinates. The point we will develop in what follows is that the phase can be found in closed form independently of the specific form of the amplitude ρ .

One key feature of NLS equations given by Eq. (1) is the conservation of the L^2 -norm $\|u\|_2 = (\int |u(x, t)|^2 d^n x)^{1/2}$ under time evolution. For self-similar solutions and choosing the norm value to be equal to one (this can be done without loss of generality by scaling appropriately the nonlinear term) this conservation law becomes

$$A^2(t) \int_{\mathbb{R}^n} (\rho(r/w))^2 d^n x = 1. \quad (8)$$

Let us choose ρ such that $\|\rho\|_2 = 1$ (this can be done without loss of generality and determines uniquely $A(t)$), then

$$A^2 w^n = 1, \quad (9)$$

thus

$$\dot{A} = -\frac{n}{2}\dot{w}. \quad (10)$$

The usual situation in applied sciences corresponds to functions for which not only the L^2 -norm is well defined (and conserved), but also the H^1 norm is well defined. In fact, the gradient term $\int |\nabla u|^2 d^n x$ is sometimes called the kinetic energy, which must be finite for physically meaningful solutions. Thus, we will look for self-similar solutions of the form (7) with finite H^1 and L^2 norms. Situations where blow-up occurs require an specific analysis near the blow-up point where $\int |\nabla u|^2 \rightarrow \infty$ [2].

Substituting (7) into (5a) gives

$$\begin{aligned} \dot{A}\psi(r/w(t)) - \frac{\dot{w}}{w^3}A(t)\psi_r(r/w(t)) = \\ - A(t)\rho_r(r/w)\phi_r(r/w) - \frac{1}{2}A(t)\rho(r/w) \left[\phi_{rr} + \frac{n-1}{r}\phi_r \right], \end{aligned} \quad (11)$$

We now define a new variable $q = r/w(t)$ and then Eq. (11) becomes, after using (10)

$$\phi_{qq} + \left(\frac{n-1}{q} + \frac{2\rho_q}{\rho} \right) \phi_q = 2\dot{w}w \left(\frac{n}{2} + \frac{\rho_q}{\rho}q \right). \quad (12)$$

It is remarkable that this is a linear second order equation whose general solution can be easily found. Defining $v(q) = \phi/(2w\dot{w})$ we get

$$v_q + \left(\frac{n-1}{q} + \frac{2\rho_q}{\rho} \right) v = \frac{n}{2} + \frac{\rho_q}{\rho} q. \quad (13)$$

The formal general solution of Eq. (13) is

$$v(q) = \frac{C_2(t)}{q^{n-1}\rho(q)^2} + \frac{q}{2}. \quad (14)$$

for any arbitrary function $C_2(t)$. Thus, integrating we get

$$\phi(q, t) = 2w\dot{w} \left[C_1(t) + C_2(t) \int^q \frac{ds}{s^{n-1}\rho(s)^2} + \frac{q^2}{4} \right]. \quad (15)$$

This is the general form of the phase of any self-similar solution to Eq. (1) with amplitude profile given by ρ . However, not all of these solutions correspond to physically interesting ones. To understand why let us compute

$$K(t) \equiv \int_{\mathbb{R}^n} |\nabla u|^2 d^n x = \int_{\mathbb{R}^n} [\rho_r^2 + \rho^2 \phi_r^2] d^n x. \quad (16)$$

As discussed above this integral (which is related to the H^1 norm of u) must be finite. However, it is clear that

$$\begin{aligned} K(t) &\geq \int_{\mathbb{R}^n} \rho^2 \phi_q^2 d^n q = \int_0^\infty \rho^2 \left[\frac{C_2(t)}{q^{n-1}\rho(q)^2} + \frac{q}{2} \right]^2 q^{n-1} dq \int_{\mathbb{S}^n} d\Omega \\ &= S_n \left[\int_0^\infty C_2(t) \left(\frac{C_2(t)}{q^{n-1}\rho(q)^2} + q \right) dq + \int_0^\infty q^{n+1} \rho(q)^2 dq \right] \end{aligned} \quad (17)$$

where \mathbb{S}^n denotes the surface of the n -dimensional sphere of unit radius and $S_n = \int_{\mathbb{S}^n} d\Omega$ is its measure. The most singular term in Eq. 17 is the first one. Taking into account that $\int_{\mathbb{R}^n} \rho^2 d^n q = 1$ we can use the Schwartz inequality to prove the divergence of the first term of Eq. (17)

$$\begin{aligned} &\left(\int_{\mathbb{R}^n} \rho^2 d^n q \right) \left(\int_0^\infty \frac{C_2(t)}{q^{n-1}\rho(q)^2} dq \int_{\mathbb{S}^n} d\Omega \right) \\ &= \left(\int_0^\infty \rho^2 q^{n-1} dq \right) \left(\int_0^\infty \frac{C_2(t)}{q^{n-1}\rho(q)^2} dq \right) S_n^2 \\ &\geq S_n^2 \int_0^\infty \rho^2 q^{n-1} \frac{C_2(t)}{q^{n-1}\rho(q)^2} dq = C_2(t) S_n^2 \int_0^\infty dq \rightarrow \infty. \end{aligned} \quad (18)$$

Which proves the divergence of $K(t)$ unless $C_2(t) = 0$. The second term in (17) cannot compensate this divergence since this would require $\rho^2 \sim 1/q^n$

for $q \rightarrow \infty$ which would lead to non-normalized solutions. Using this fact and changing back to physical variable r we get finally for the phase

$$\phi(r, t) = \frac{\dot{w}}{2w} r^2. \quad (19)$$

Eq. (19) is one of the main results of this paper: *the phase of finite-energy self-similar solutions is quadratic* irrespective of the many possible variations of the problem (nonlinearity, potential, spatial dimensionality). This fact explains why the choice of quadratic phases as in (6) in time-dependent variational method leads to very good results. This fact also clarifies why these approximate methods lead usually to a prefactor $\beta = \dot{w}/(2w)$, which is indeed the exact result.

We must emphasize that phase choices such as (19) have been used previously by other authors either as approximate expressions for the phase as commented before or as an specific choice leading to particular solutions (e.g. in the framework of the theory of self-focusing in NLS equations [2,16]). What we prove here is that *all finite-energy self-similar solutions to Eq. (1) must have a quadratic phase*, which is a stronger result.

2.2 Equations for the scaling parameter

When self-similar solutions (or quasi-solutions in the sense discussed above) are considered it is possible to get closed equations for the evolution of the most relevant parameter $w(t)$ which determines the width of the solutions. In this section we restrict ourselves to the autonomous case when V and g do not depend explicitly on t . Let us first consider the hamiltonian

$$H = \frac{1}{2} \int |\nabla u|^2 d^n x + \int G(a^2) d^n x + \int V(x) |u|^2 d^n x, \quad (20)$$

where G is a real function satisfying $g = \partial G / \partial(a^2)$. It is easy to check that H is a conserved quantity which is assumed to be finite. For self-similar solutions of the form (7) and using again the definition $q = r/w$, we get

$$\begin{aligned} H &= \frac{1}{2} \int_{\mathbb{R}^n} \left(\left| \frac{\partial \rho}{\partial r} \right|^2 + \rho^2 \left| \frac{\partial \phi}{\partial r} \right|^2 \right) d^n x + \int_{\mathbb{R}^n} G(A^2 \rho^2) d^n x + A^2 \int_{\mathbb{R}^n} V(x) \rho^2 d^n x \\ &= \frac{1}{2} A^2 w^n \int_{\mathbb{R}^n} \left(\frac{\rho_r^2}{w^2} + \frac{\rho^2}{w^2} \phi_q^2 \right) d^n q + w^n \int_{\mathbb{R}^n} G \left(\frac{\rho^2}{w^n} \right) d^n q \\ &\quad + \int_{\mathbb{R}^n} A^2 w^n V(wq) \rho^2 d^n q. \end{aligned} \quad (21)$$

Using the L^2 -norm constraint (9) we get

$$H = \frac{1}{2w^2} \int_{\mathbb{R}^n} \rho_q^2 d^n q + \frac{1}{2w^2} \int_{\mathbb{R}^n} \rho^2 \phi_q^2 d^n q + w^n \int_{\mathbb{R}^n} G(\rho^2/w^n) d^n q + \int_{\mathbb{R}^n} V(wq) \rho^2 d^n q. \quad (22)$$

Finally, we use (15) and the fact that

$$\int_{\mathbb{R}^n} d^n q = \int_0^\infty q^{n-1} dq \int_{\mathbb{S}^n} d\Omega \equiv S_n \int_0^\infty q^{n-1} dq, \quad (23)$$

to get

$$\begin{aligned} \frac{H}{S_n} &= \frac{1}{2w^2} \int_0^\infty \rho_q^2 q^{n-1} dq + \frac{1}{2} \dot{w}^2 \int_0^\infty \rho^2 q^{n+1} dq \\ &+ w^n \int_0^\infty G(\rho(q)^2/w^n) q^{n-1} dq + \int_0^\infty V(wq) \rho^2 q^{n-1} dq. \end{aligned} \quad (24)$$

Differentiating (24) with respect to time we obtain

$$\begin{aligned} & - \frac{\dot{w}}{w^3} \int_0^\infty \rho_q^2 q^{n-1} dq + \dot{w} \ddot{w} \int_0^\infty q^{n+1} \rho^2 dq + n w^{n-1} \dot{w} \int_0^\infty G(\rho^2/w^n) q^{n-1} dq \\ & - w^n \int_0^\infty \frac{n w^{n-1} \dot{w}}{w^{2n}} \rho^2 g(\rho^2/w^n) q^{n-1} dq + \int_0^\infty V'(wq) q \dot{w} \rho^2 q^{n-1} dq = 0, \end{aligned} \quad (25)$$

which can be written as a Newton-like equation

$$\left(\int_0^\infty q^{n+1} \rho^2 \right) \ddot{w} = \frac{\left(\int_0^\infty q^{n-1} \rho_q^2 dq \right)}{w^3} \quad (26a)$$

$$- n w^{n-1} \int_0^\infty \left[G\left(\frac{\rho^2}{w^n}\right) - \frac{\rho^2}{w^n} g\left(\frac{\rho^2}{w^n}\right) \right] q^{n-1} dq \quad (26b)$$

$$- \int_0^\infty q^n V'(wq) \rho^2 dq. \quad (26c)$$

The different terms in Eq. (26) have a very clear physical interpretation. The right-hand-side of Eq. (26a) is a repulsive term proportional to $1/w^3$ which accounts for the tendency of the wave-packet to spread under the action of dispersion (this is mathematically described by the term with the Laplacian in Eq. (1)). The second one (Eq. (26b)) is the self-interaction energy due to the nonlinearity. Finally the last term given by Eq. (26c) comes from the interaction with the external potential V .

Eqs. (26) are of the same form as the equations arising in particular studies of Eq. (1) based on the method of collective coordinates of which Eqs. (26) are a generalization. From them it is possible to understand that when self-similar solutions exist what the variational method does is to fit somehow the right dynamics but using different values for the integrals depending on ρ .

Due to the lack of knowledge of the right self-similar profiles ρ , the integrals are estimated by using the ansatz φ . If the ansatz is constructed reasonably, e.g. taking into account the right asymptotic behavior of the solutions, we may expect only a quantitative discrepancy between the exact results for self-similar solutions and the estimates obtained from the collective coordinate method obtained from Eq. (26).

The main advantage of our derivation of Eqs. (26) is that they are obtained systematically on the basis of the exact phase of self-similar solutions. These equations provide then a direct way to obtain estimates for the dynamics when self-similar solutions do not exist and allow to avoid the lengthy calculations of the method of collective coordinates.

There is a lot of information contained in Eqs. (26). Specifically, they describe many cases previously studied. For instance, the simplest case $g(y) = g_0 y^2, g_0 < 0, V = 0$ corresponds to the usual focusing cubic NLS. From there we obtain immediately the following condition for the collapse of self-similar solutions

$$g_0 < g_c = -\frac{\int_0^\infty (\rho_q)^2 q^{n-1} dq}{\int_0^\infty q^{n-1} \rho^4 dq} \quad (27)$$

which allows to estimate the critical value of g for solutions with $\|\rho\|_2 = 1$. For instance taking gaussians one gets $g_c = -2\pi$, which is the usual estimate obtained from time-dependent variational methods. Taking ρ to be the so-called Townes-soliton [2] leads to the exact result for the critical value of g [2].

Many other situations have been described in the literature. Taking $V(r) = \frac{1}{2}\Omega^2 r^2$ and $g(y) = g_0 y^2, g_0 \in \mathbb{R}$ we get the simplest situation of Bose-Einstein condensation in a symmetric trap. This problem was studied variationally in Ref. [17]. Our equations coincide with those for the spatially symmetric case discussed there. Also in Refs. [18,19,20] cubic-quintic nonlinearities were used to describe four-body collisions in Bose-Einstein condensates. Eqs. (26) give us the evolution equations found there by just choosing a nonlinearity of the type $g(y) = g_3 y^2 + g_5 y^4$.

3 Conclusions and discussion

In this paper we have studied the phase of self-similar solutions to general Nonlinear Schrödinger equations. Our analysis provides a better understanding of the way collective coordinate methods work. Also we have used the results on the phase to find an effective equation describing exactly the dynamics of self-similar solutions to the NLS equation and approximating the dynamics of other, more complicated solutions.

Our analysis on the phase can be easily extended to more complicated vector systems. We expect that the procedure followed here may provide a basis for choosing systematically the phase for more complex ansatzs such as those which are not self-similar thus overcoming one of the difficult points of usual collective coordinate methods. It is worth mentioning that our analysis of the phase is applicable to non-autonomous situations such as the ones recently discussed in Refs. [21,22,23,24,25], which represent an emerging field of applications of Nonlinear Schrödinger Equations.

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